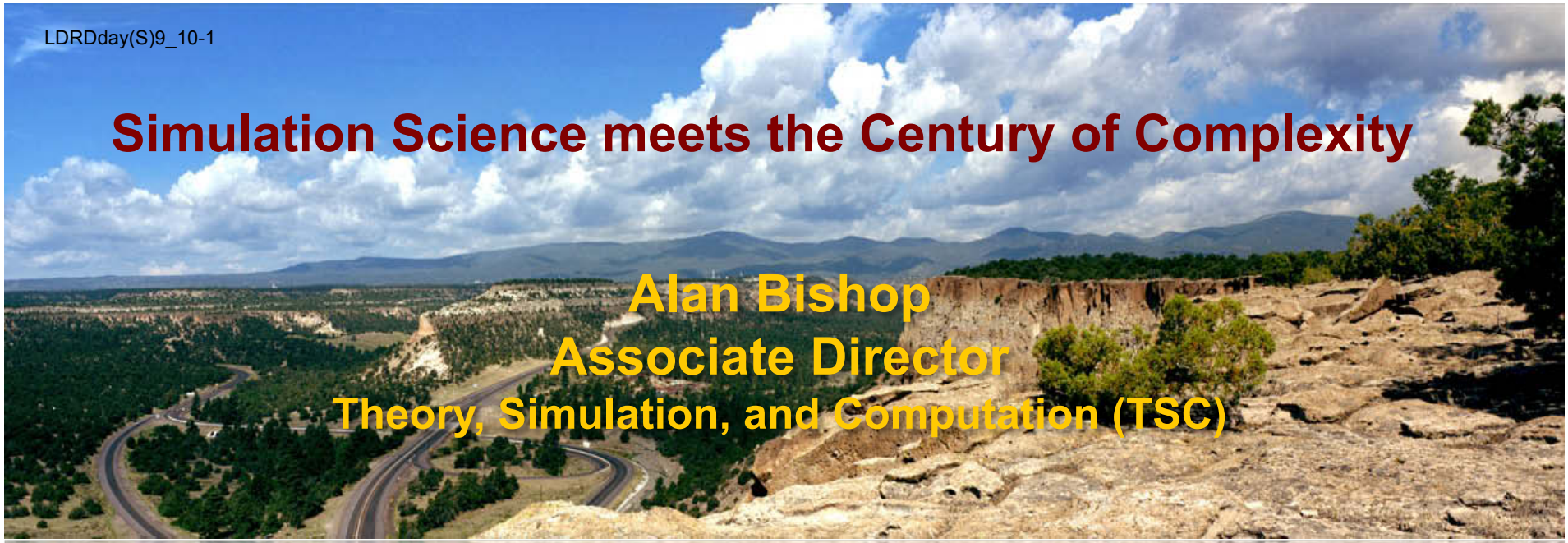


Simulation Science meets the Century of Complexity

Alan Bishop
Associate Director
Theory, Simulation, and Computation (TSC)

- "High-Performance" Computing and Visualization have come of age as tools in the "Scientific Method" for very Complex Systems
- A "Perfect Storm" of need and opportunity over the next decade to face international Energy, Security, Health,…imperatives: Understanding, Prediction, Management
- "Co-Design" of S&T assets essential to accelerate discovery to application

Los Alamos NATIONAL LABORATORY EST.1943
Operated by Los Alamos National Security, LLC for NNSA

UNCLASSIFIED LA-UR 10-05881

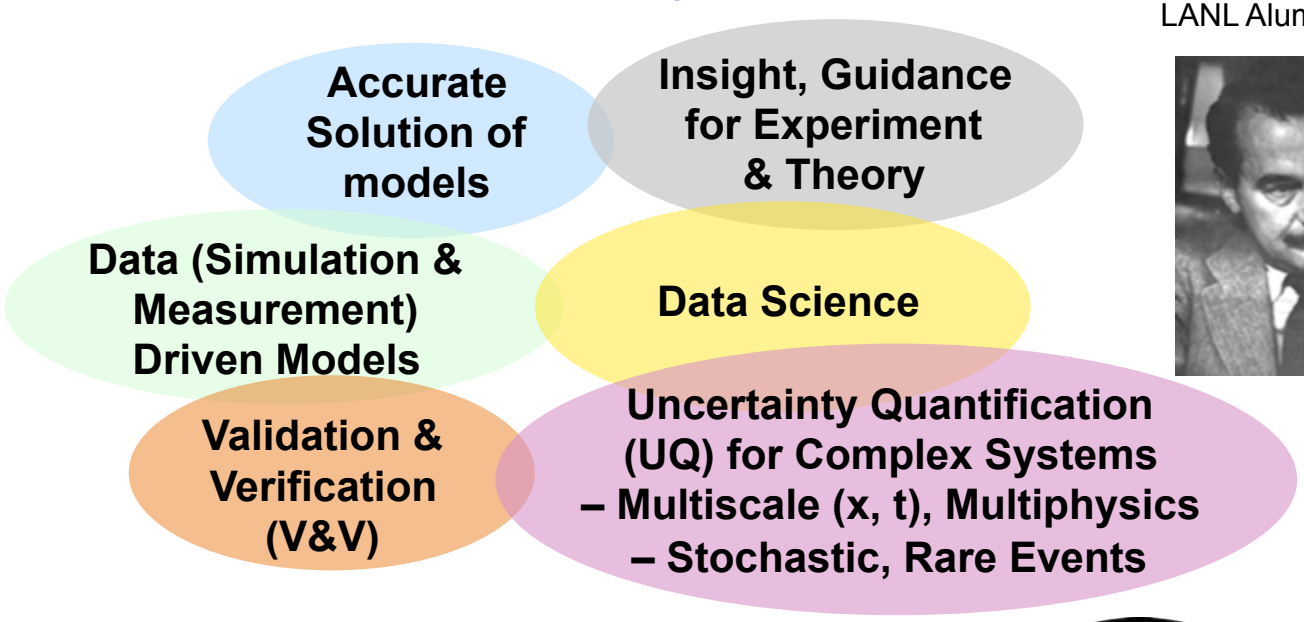
Acknowledgments:
DOE-ASCR http://www.er.doe.gov/ascr/
A. White and other LANL colleagues

NNSA

High-Performance/Advanced/Super Computing and Visualization

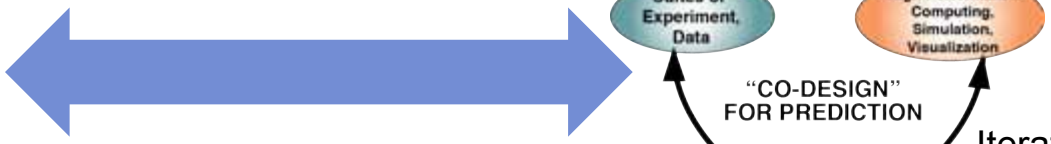
- A "NEWly" mature scientific capability for the scientific method
- Many leaders emerged from traditional disciplines (Physics, Mathematics….); Increasingly an identified discipline at Universities (Computer Science…)

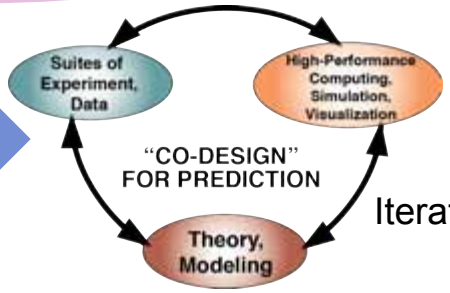
?HPC?



LANL Alumni

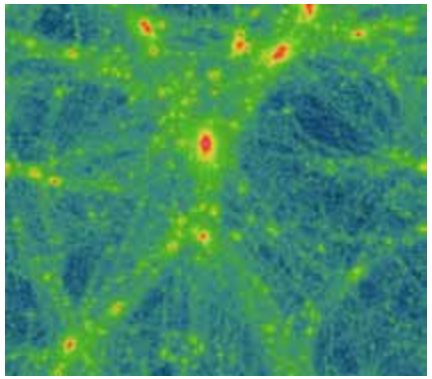
Robust Tools for Decision Makers





Iterate to Success!

"The Century of Complexity" (S. Hawking)



Cosmology: Filaments, Clusters, and Voids

Science @ Scale

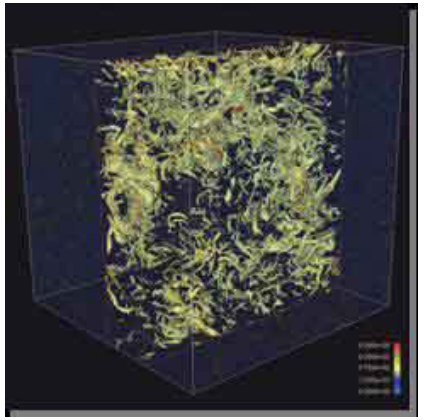
Systems of connected functional scales in space, time; Emergent functions; Extreme conditions

Enabled by huge advances in Data, Simulation, Nonlinear Science…

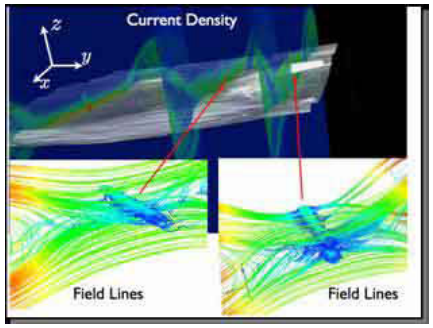
BUT…

? Origins, Measures, Consequences ?

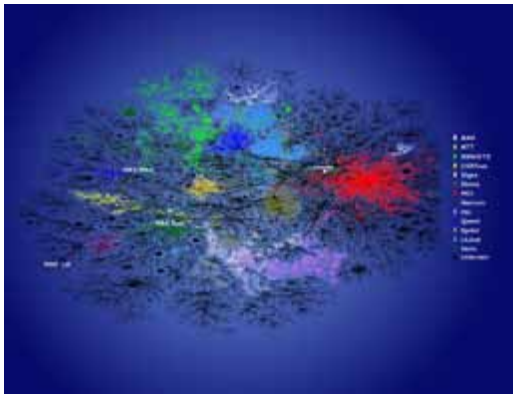
Multiscale Modeling, Simulating, Measuring ≠…at Multiple Scales: Need IS&T



Fluid Turbulence

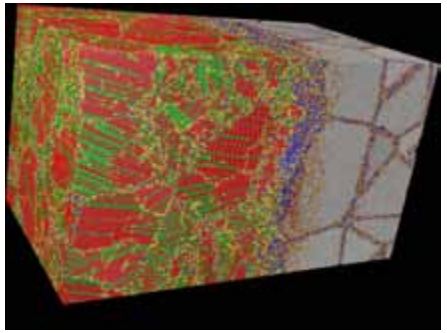


Magnetic Reconnection



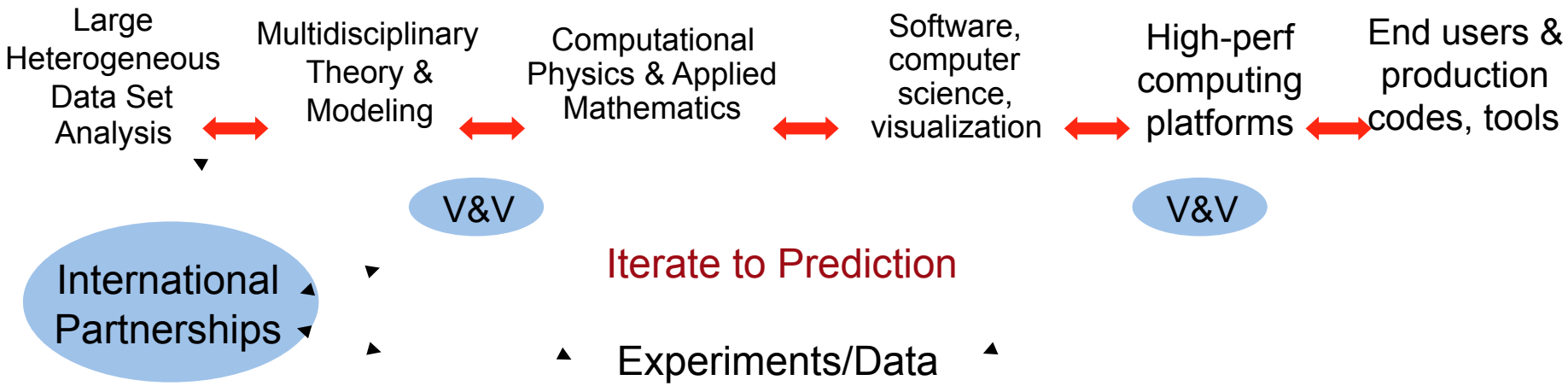
Communication Networks

Protein Dynamics



Shocked Metals

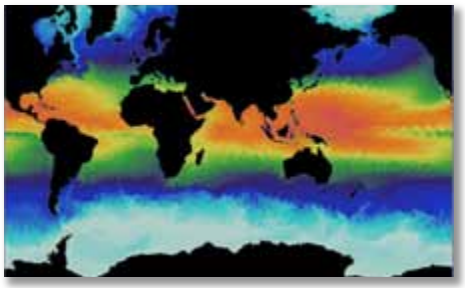
Integration Capability … a nuclear weapons heritage of 65+ years



Central to the huge national need for new generations of ideas, concepts and methodologies to improve the fidelity, reliability, certainty, and usability of tools to guide and interpret experiments, and provide prediction and control for complex phenomena and systems.

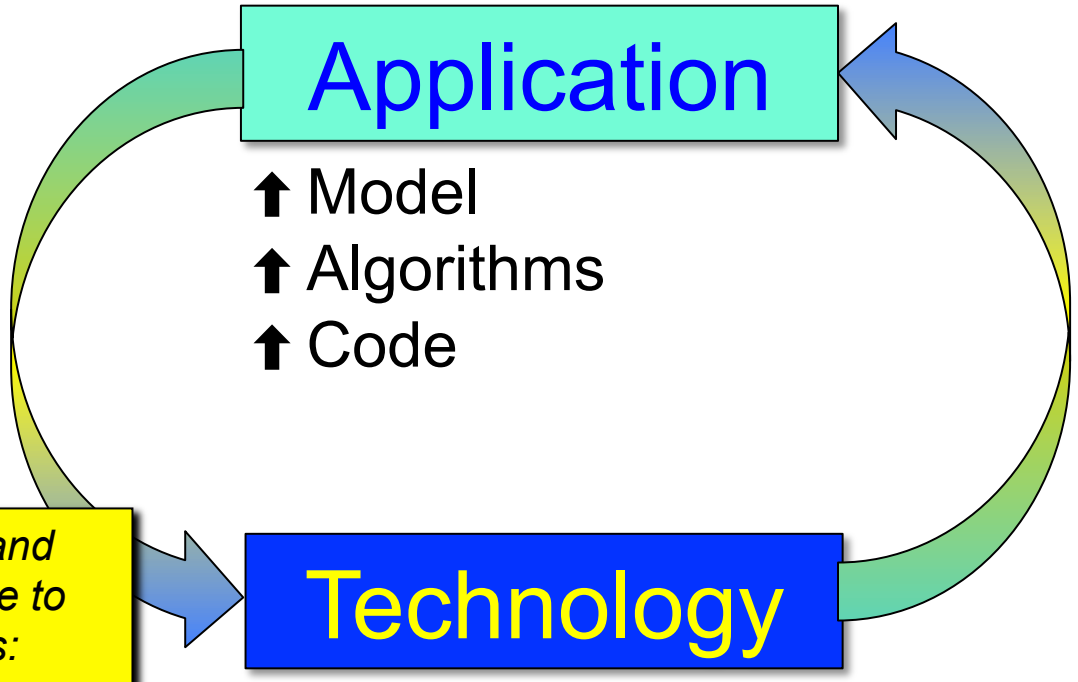
DOE mission imperatives require simulation and analysis for system understanding, prediction, policy and decision making

- ***National Nuclear Security*: Maintaining a safe, secure and reliable nuclear stockpile**
  - Stockpile certification and management
  - Predictive scientific challenges
  - Real-time evaluation of urban nuclear detonation
- ***Climate Change*: Understanding, mitigating and adapting to the effects of global warming**
  - Sea level rise
  - Severe weather
  - Regional climate change
  - Geologic carbon sequestration
- ***Energy*: Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production**
  - Reducing time and cost of reactor design and deployment
  - Improving the efficiency of the existing light water reactor fleet
- ***Materials*: Understanding and design of materials in extreme conditions**
  - Predictive multi-scale materials modeling: observation to control
  - Effective, commercial technologies in renewable energy, catalysts, and batteries



HPC and IMPACT: beyond traditional one-sided approaches essential: "Co-Design" opportunity during "disruptive" technology transition

Application driven:
Find the best technology to run this code.
Sub-optimal

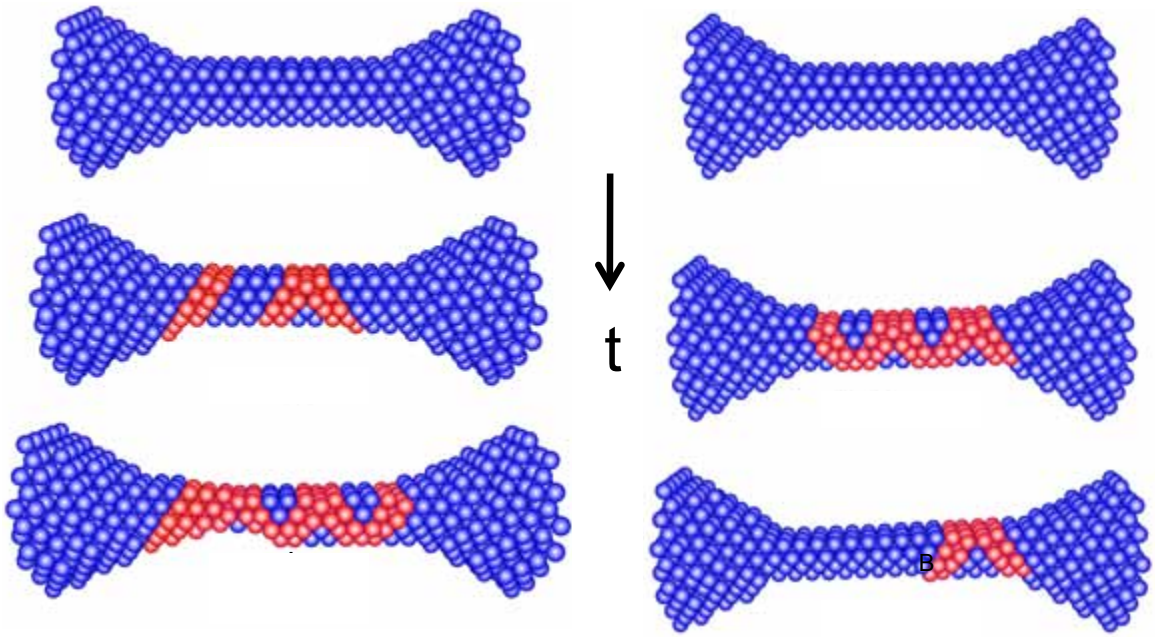


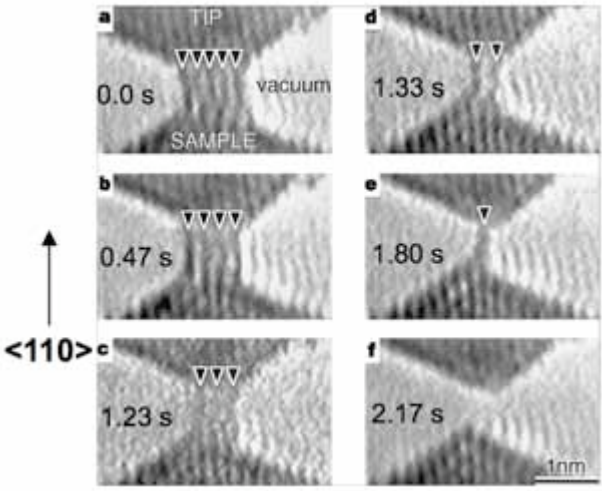
Best
Power?
Performance?
Price?
Prediction?
Productivity?

Now, we must expand the co-design space to find better solutions:
- *new applications & algorithms,*
- *better technology and performance.*

Technology driven:
Fit the application to this technology.
Sub-optimal.

Using Roadrunner Cell architecture for accelerated dynamics: atomistic simulations long enough to be directly validated by experiment





(note rotated orientation)

High strain rate simulation shows necking

Lower strain rate simulation thins uniformly

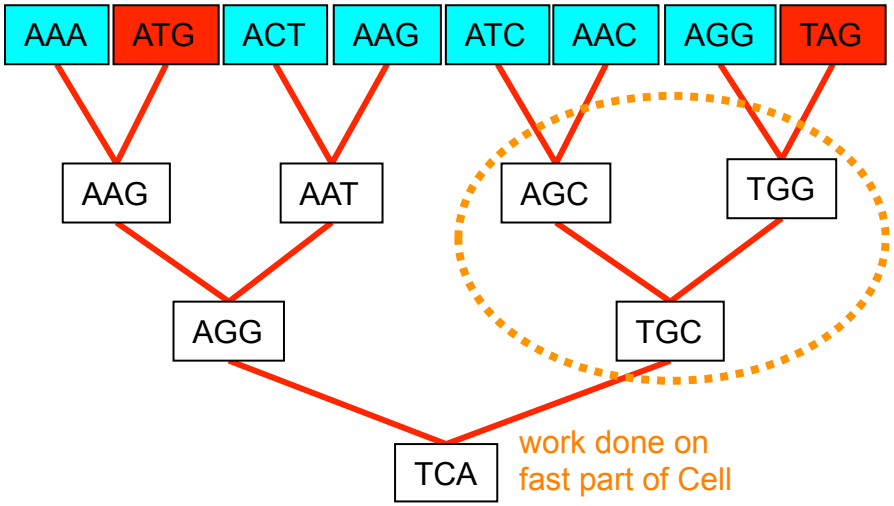
Gold nanowire experiment (STM) can be compared with Roadrunner simulations

Stretching Metallic Nanowires (for strength, transport….)

(Pao, Perez, Swaminarayan and Voter)

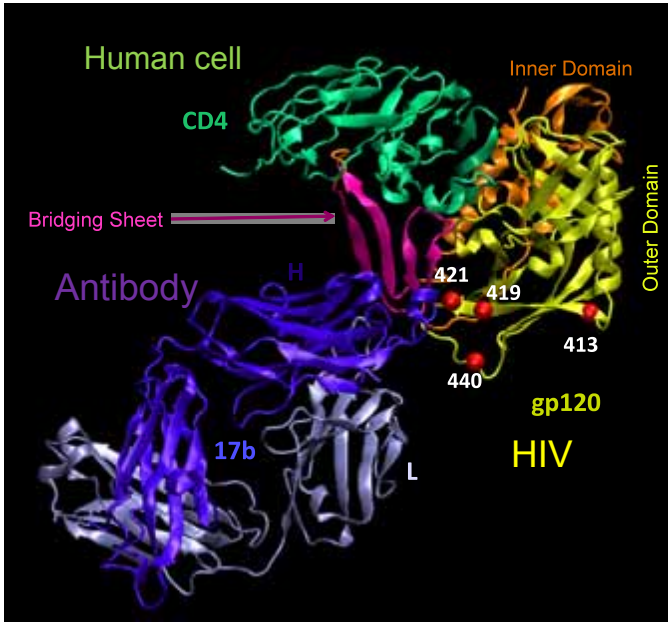
Using Roadrunner Cell Architecture for Viral Phylogenetics: Inheritance vs. Adaptation? HIV Vaccine design?

Seeking correlation patterns of HIV viruses that are immunologically potent; infer "family tree" of > 4,000 HIV sequences (10^4 nucleotides each)



> 10^5 CPU hours on Roadrunner
Huge # matrix inversions

HIV Vaccine Implications?



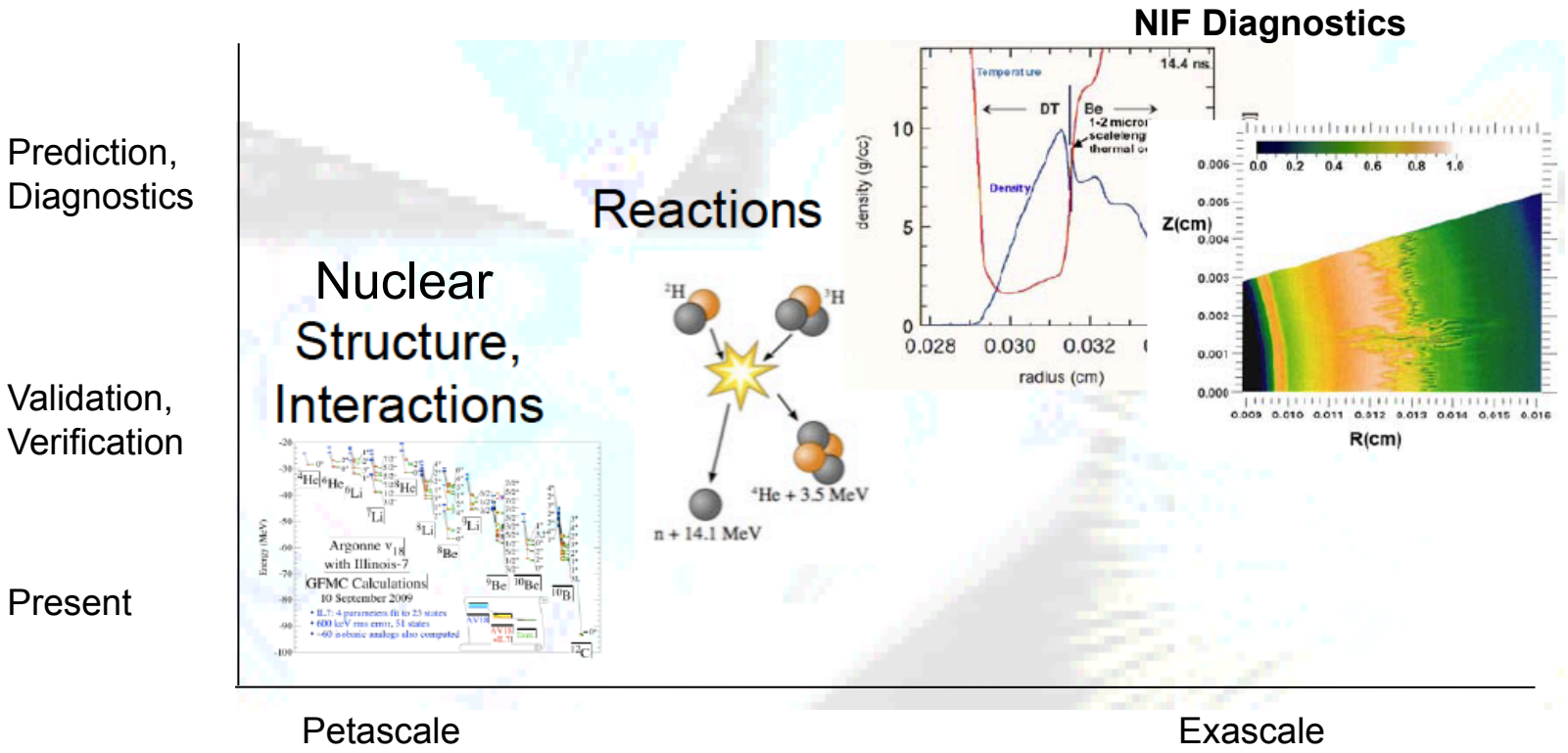
- CD4i region of viral envelope important for good immune response (inducing antibodies).
- Experiments underway to verify.

(T. Bhattacharya et al)

!...and next Exascale (10^{18} flops/sec) by 2018…!

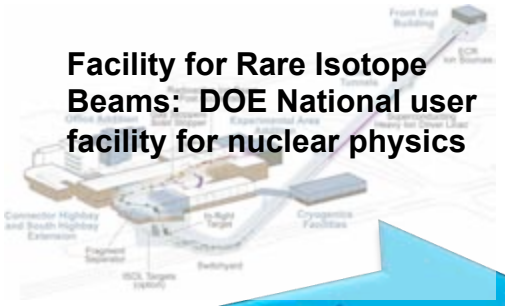
e.g. Fusion (Thermonuclear Reactions)

Drivers: Using nuclear reactions to diagnose complex High Energy Density environments (National Ignition Facility; Astrophysical…)

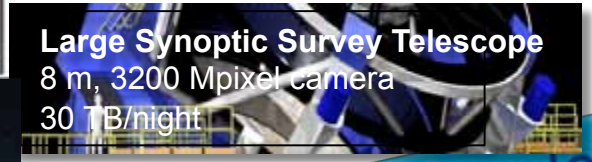


(from National Security Workshop (10/09)
http://www.er.doe.gov/ascr/

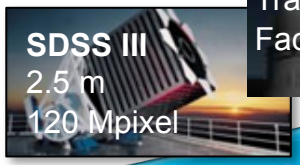
Supernovae



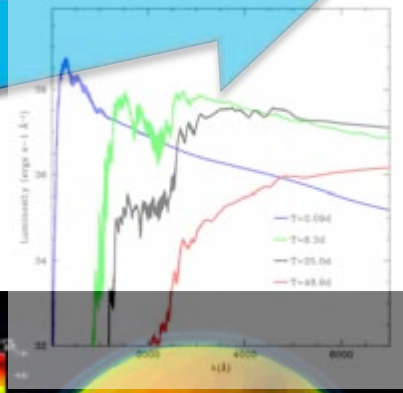
Facility for Rare Isotope Beams: DOE National user facility for nuclear physics

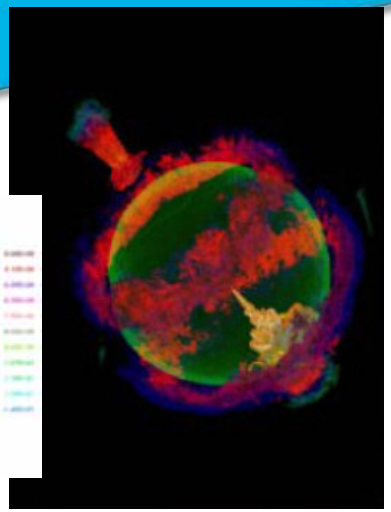


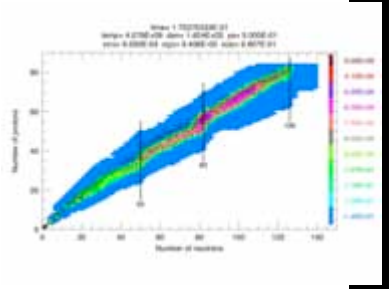
Palomar Transient Factory



Supernovae: Probing Cosmology, Nuclear and Particle physics

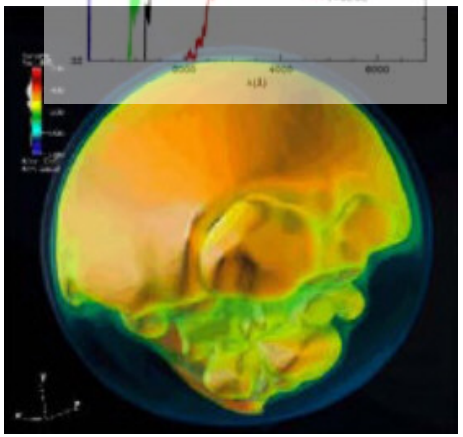






"HPC allows the inclusion of the physics needed to solve these problems (burning fronts, multi-dimensional transport of neutrinos and photons, nuclear and particle physics)"

• **Exascale** – will allow 3D high-resolution, full (multi-angle) transport, advanced opacities: **Can relate explosion mechanisms (and nuclear and particle physics) directly to the observed data!**



2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020

10 PF/sec — 100 PF/sec — EXASCALE

From **"The Physics of Materials, How Science Improves our Lives"**
National Academy Press, 1999

- "…. today our challenge is to extend that understanding to more **complex** forms of matter - and to more **complex phenomena** … **a whole new style of inquiry** …"

- "It is becoming increasingly **interdisciplinary**, with progress often being made at the interfaces of biology, chemistry, materials science, and atomic and molecular physics."

- "A community more closely connected with industry and with the rest of science and **armed with experimental and computational capabilities that were not even imaged just a few decades ago."**

"Systems Biology/Quantitative Biology"

http://www.icsb2001.org/what_is.html

The goal of Systems Biology is the construction and experimental validation of models that explain and predict the behavior of biological systems…. Characterized by a synergistic **integration of theory, computation, and experiment.** Only through this inter-disciplinary approach can we achieve a multiscale, multiresolution understanding of complex biological processes.

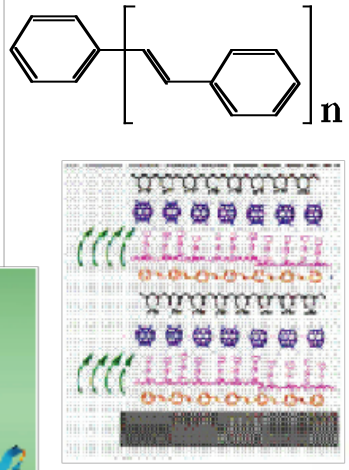
Functional Multiscale Complexity in "Tunable Electronic Matter"

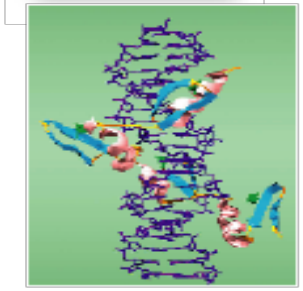
From poorly informed idealizations

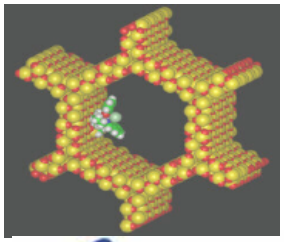
(1980)

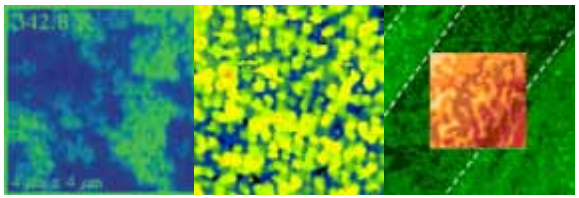
Better "Cooking & Looking"

(2000)

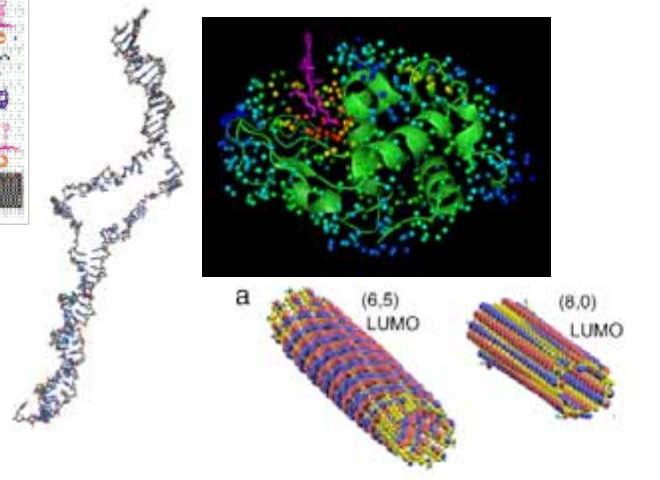








VO2 MIT (NFOM) | Gap in HighTc (STM) | CMR domains (MFM)



Need better Cooking, Looking, Simulating AND INTEGRATION

Observing & Controlling Intrinsic Complexity

Coupled
Spin-Charge-Ion

⬇

Strongly correlated, intrinsically soft, multiscale, glassy

- **Correlated "Hotspots"**
- **Adaptive phases**
- **Aging, Healing, Training**

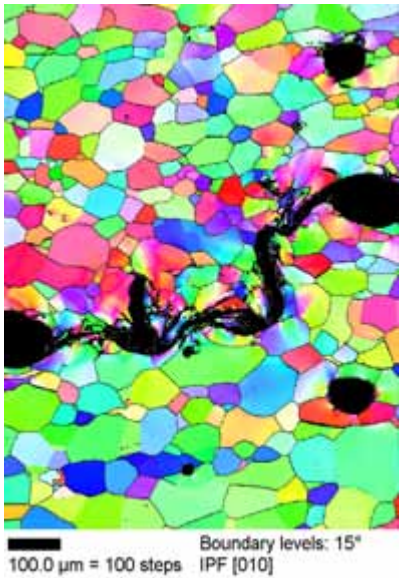
⬇

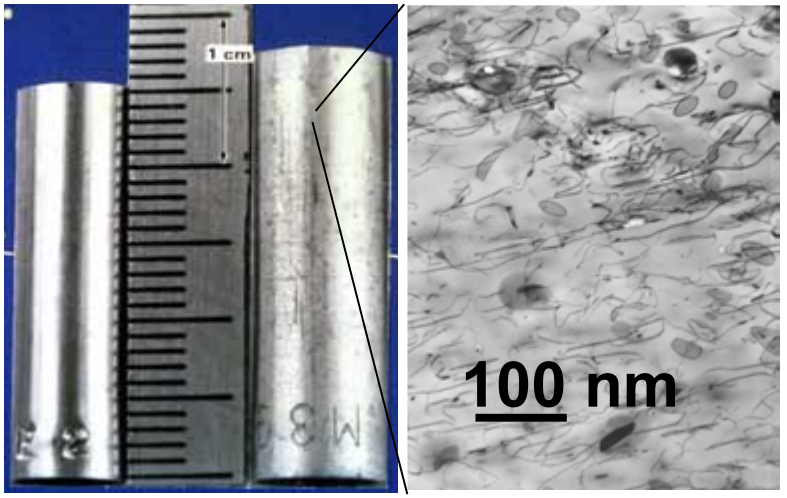
Systems/Networks of connected, functional scales (structural and electronic)

Los Alamos NATIONAL LABORATORY EST.1943

The "micron frontier": Bridging the gap between atomic understanding and bulk performance

~ 1 μm is the domain of defect consequences and microstructure interactions that drive materials strength, damage evolution, etc.

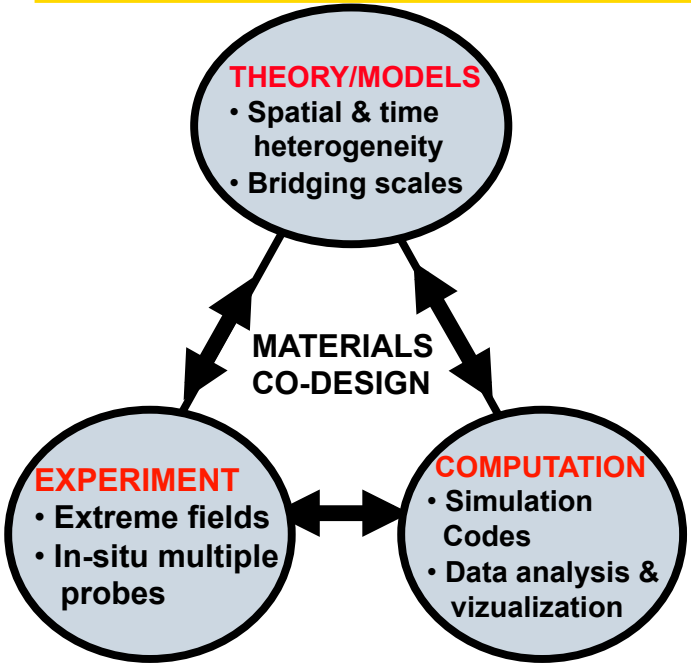


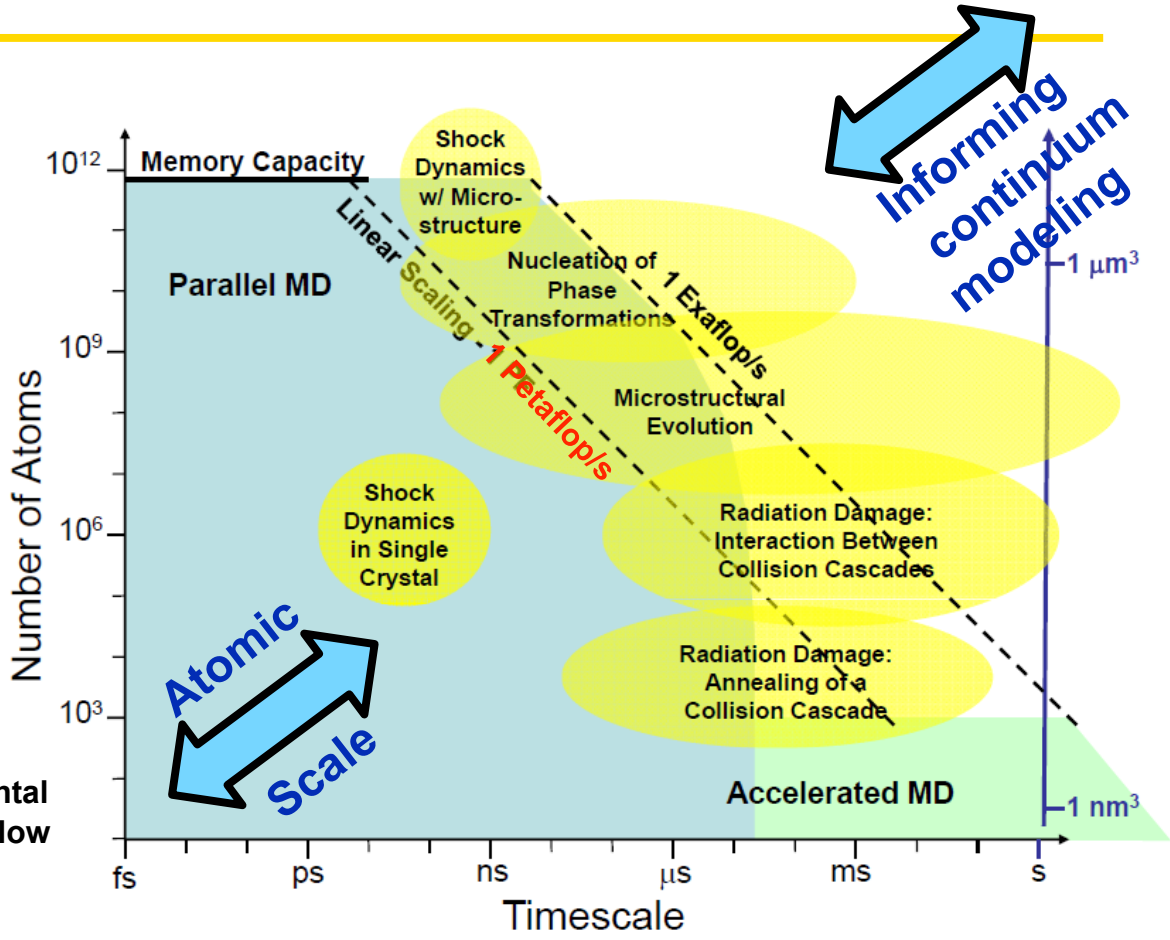


Dynamic, stochastic, rare processes in extreme environments dominate the phenomena that we do not understand

MaRIE will be the first capability with unique co-located tools necessary to realize transformational advances in materials performance in extremes

A Decadal Opportunity for Materials Science:
Removing Key Scientific Barriers to Discovery, Prediction and Control

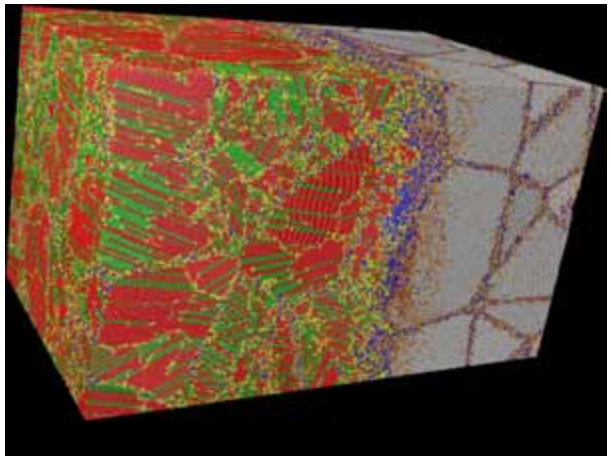




Anticipated advances in modeling, petaflop–exaflop computing, and experimental tools with unprecedented resolution, will allow access to rate-limiting phenomena at the meso (micron) scale

MaRIE: Matter-Radiation Interactions in Extremes
LANL Signature Facility plan (NW, NE, Fission-Fusion…)

e.g., Quantifying Molecular Dynamics Studies with Information Science and Technology Tools



K. Kadau et al., *Phys. Rev. Lett.* (2006).

Shock-induced transformation in Fe predicted by large-scale molecular-dynamics simulations

bcc (gray)->comp bcc (blue)->hcp,fcc (red,green)

Simulations consistent with experiment: ultrafast (nanosecond) X-ray diffraction (shocks and high intensity X-rays produced by high energy laser systems OMEGA/ Janus/Vulcan)

D.H. Kalantar et al., *Phys. Rev. Lett.* (2005).

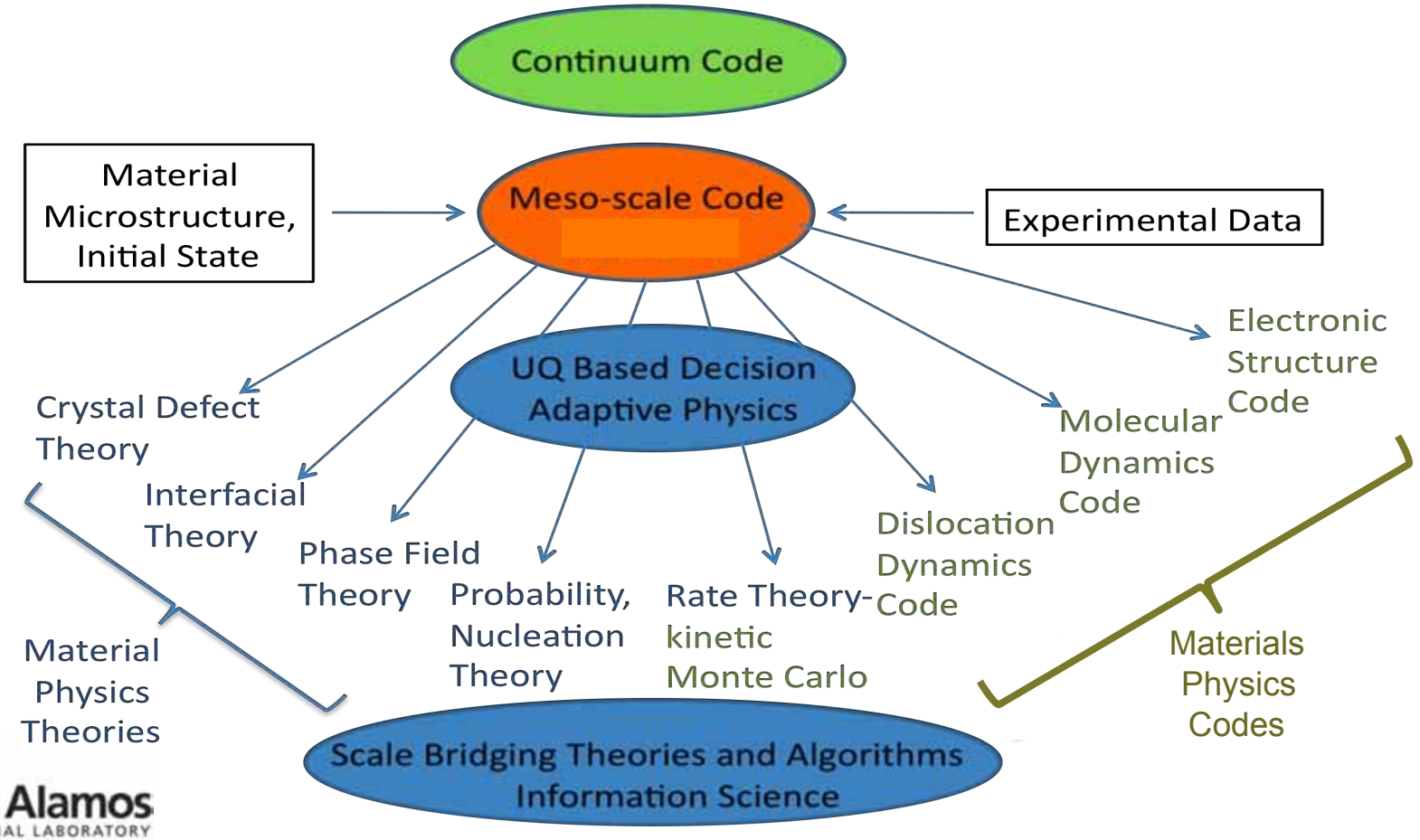
(Kober et.al)

- Massive MD studies:
  Trillions of atoms = several cubic microns
- Tool to characterize sensitivity to polycrystalline morphology, realistic defect concentrations: However, massive data sets with limited storage capacity
- Use IS&T to identify "interesting" events in real time and save additional information in those areas: machine learning, etc, for anomaly detection and classification
- More quantitative description of local geometry: phase transitions, slip planes, dislocation loops, etc.
- Intelligent coarse-graining for reduced order, stochastic modeling: basis for larger scale models (e.g. plastic flow).
- Test sensitivity of results to the form and parameters of potential functions.
- Comparison and iteration with experimental results!

i.e. address throughput/volume of observational and simulation data with automated "real-time" data analysis, UQ and parameter extraction, advanced database methodologies.

Co-Design for High Fidelity Adaptive Materials Simulation

- **Bridging of methods for high fidelity prediction with quantified accuracy and uncertainty**
- **Direct multi-scale embedding of sub-scale simulation into coarse scale simulation**
- **Combining real-time, adaptive computational AND physics methods**



MaRIE: Matter-Radiation Interactions in Extremes
LANL Signature Facility plans for Control Science

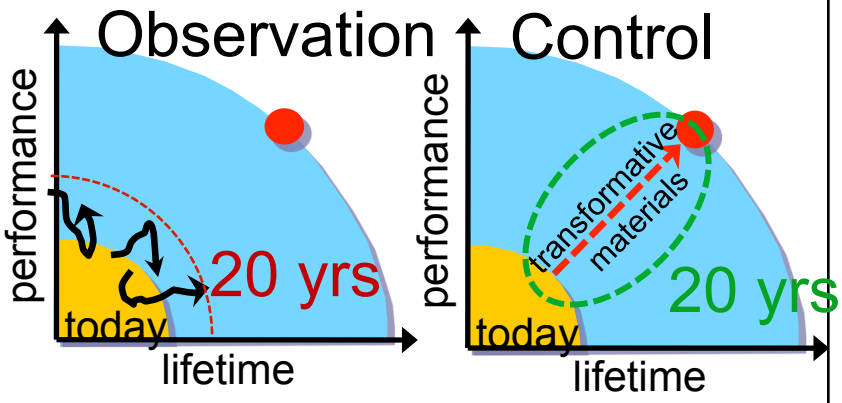
(J. Sarrao et al)

Challenges for Materials in Extremes

Radiation - *Radiation damage, Photovoltaics*
Dynamic - *Stockpile certification, Detonation propagation*
Chemical, electric and magnetic fields - *Energy storage, Superconductivity*

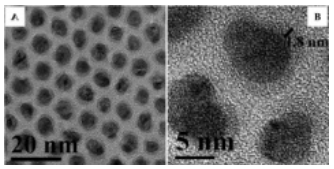
Control Science

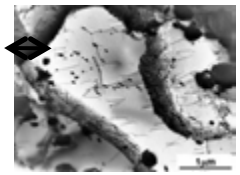
Accelerated materials discovery



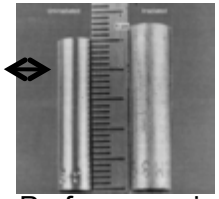
Integration - key to prediction of material properties

Theory and models that take function to structure
Synthetic control of defects and interfaces
Characterization of the evolution of defects and interfaces in multiple extremes to provide feedback





Mesoscale microstructure



Performance in Extremes

MaRIE - Control Science in Extremes

F^3
In Situ
Irradiation

User Interface

MPDH
X-ray Movies
Dynamic Extremes

NHMFL

M4
Controlled Synthesis
Non-destructive n-D Characterization
Lab-scale Extremes

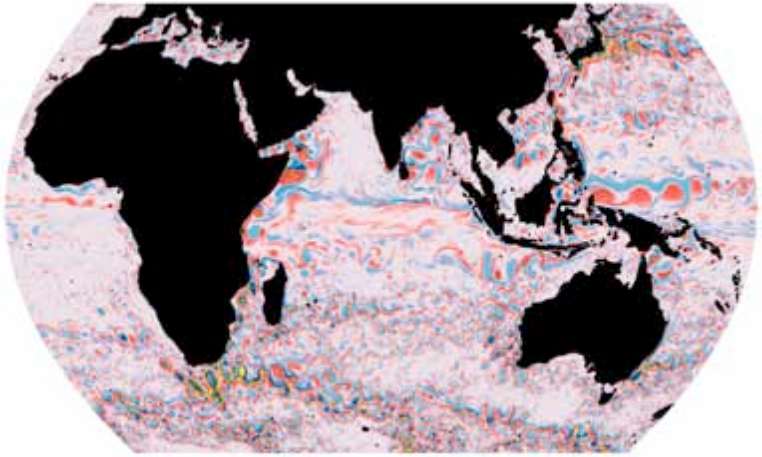
Enhanced Lujan

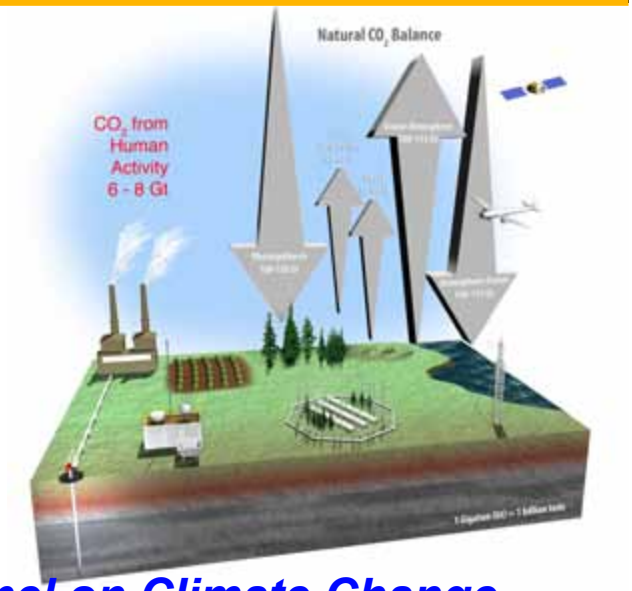
Theory/ Modeling
Roadrunner

CINT

Integrated Material Solutions
Performance in Extremes

Global Climate Science: Tools for Policymakers

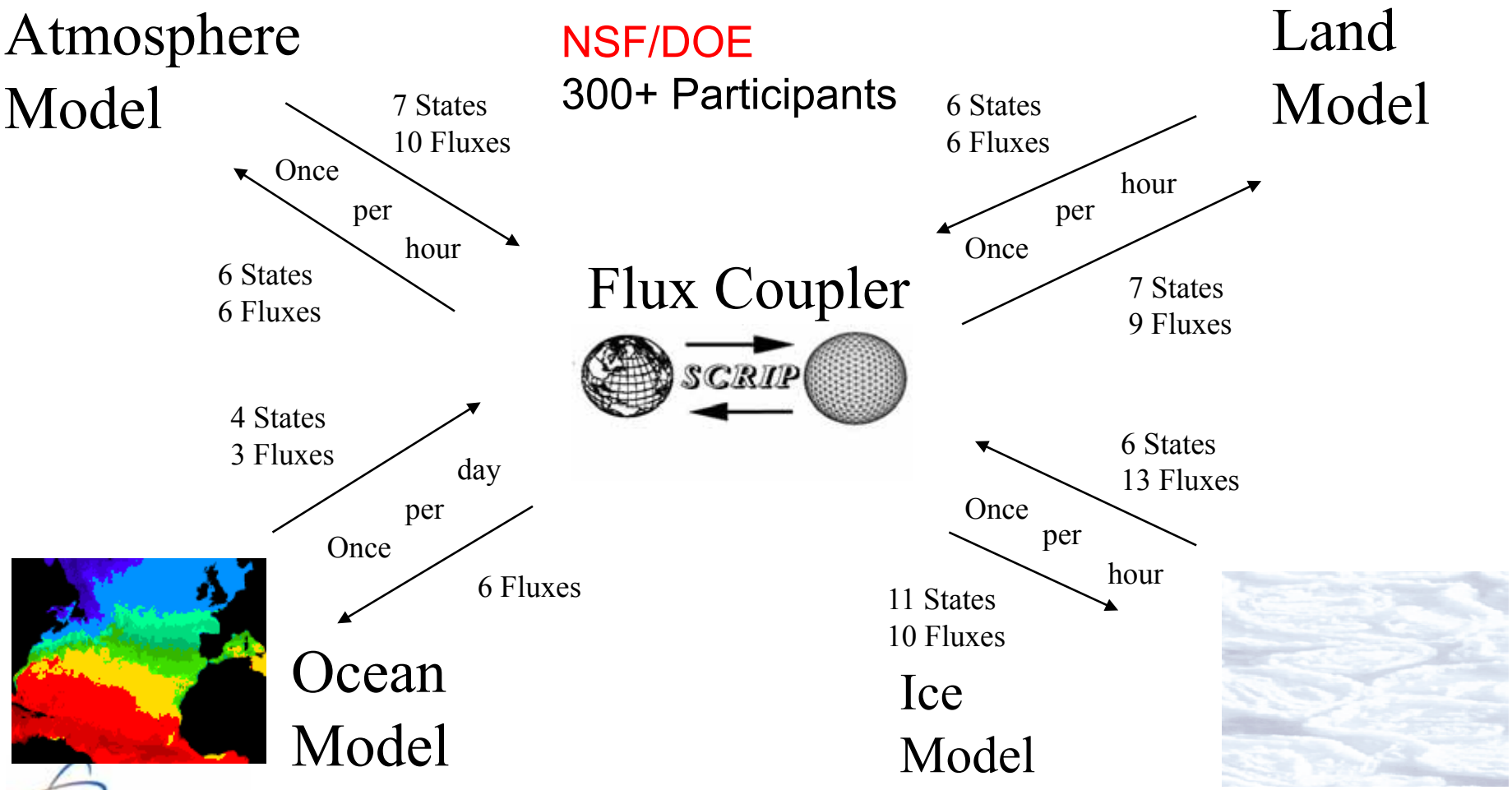




- **Los Alamos developed the Coupled Sea-Ice Model:** ***the global standard used by the Intergovernmental Panel on Climate Change***
- **Los Alamos makes key contributions to the DOE/NSF Community Climate System Model:** ***the first interactive model of molecular to planetary scale***
- **National Challenge*: Science-based policies for energy use, regional infrastructure investments, and resource allocation***

Understanding climate change as a global system is required to develop predictive tools for mitigating regional impacts

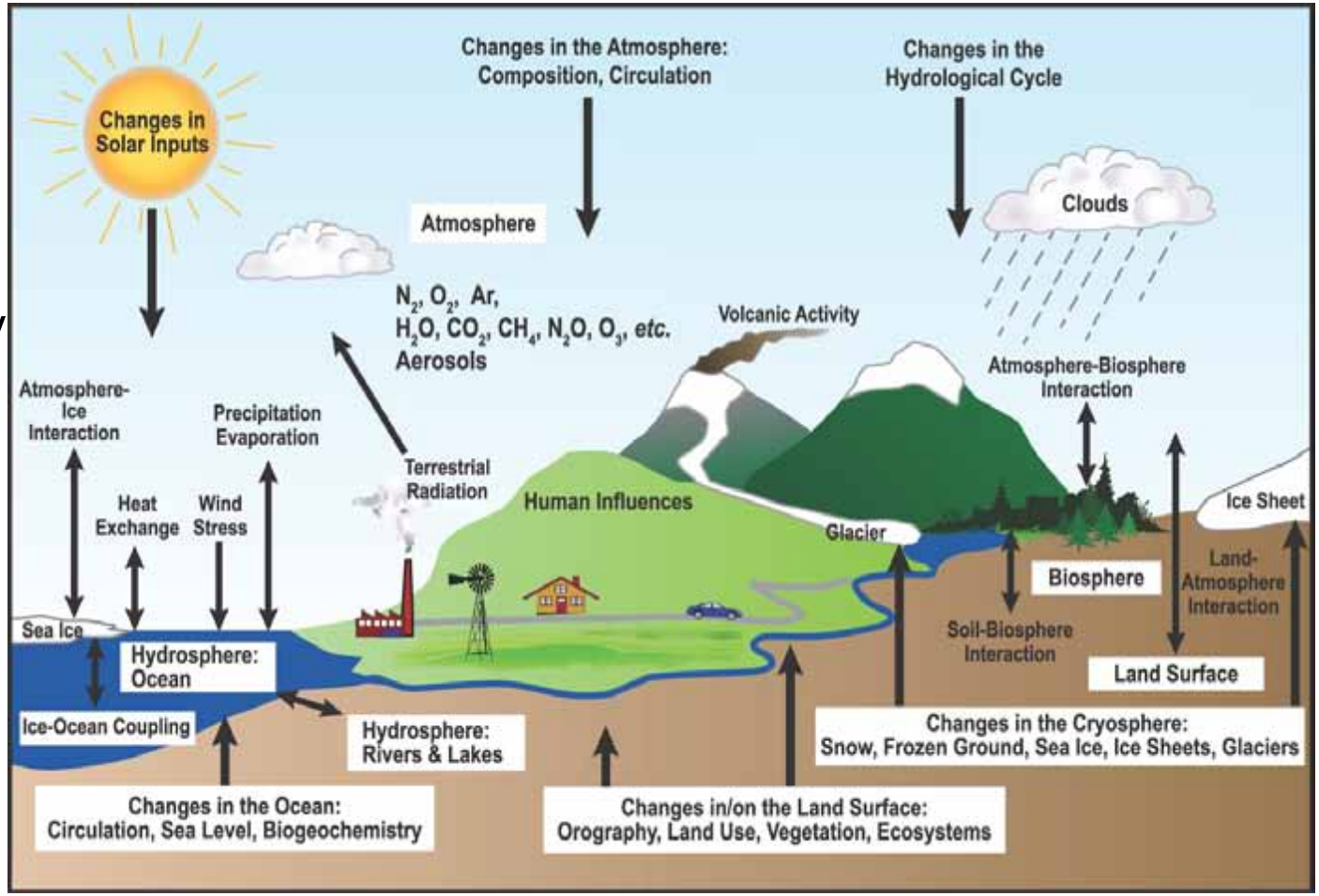
The Community Climate System Model: Co-Design and Collaboration



Climate details are complex!

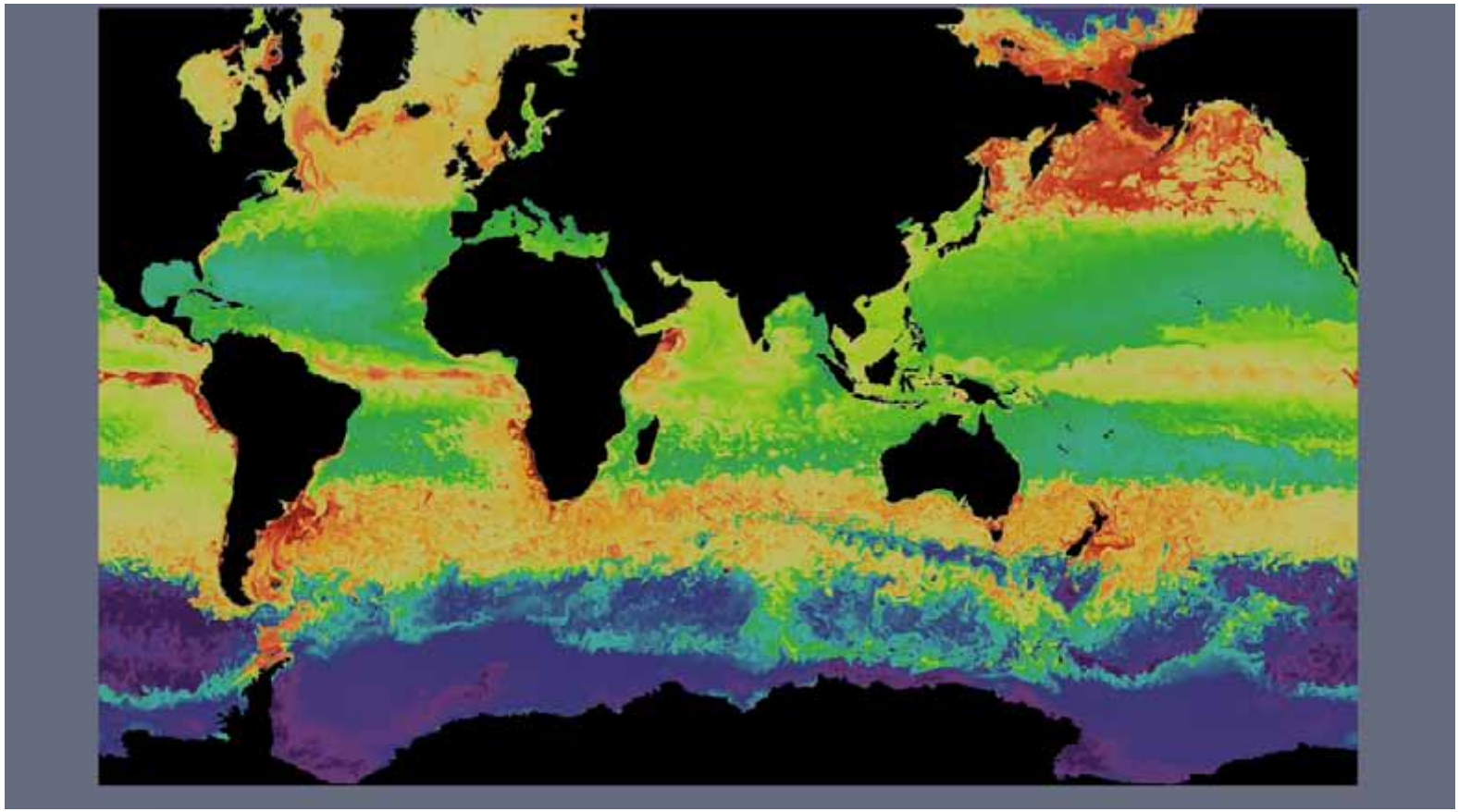
Coupled
Dynamics
Physics
Biogeochemistry

Human
Interactions



e.g., Eddy-resolving Ocean Modeling: a tour-de-force of Computational physics, Computer science, and HPC

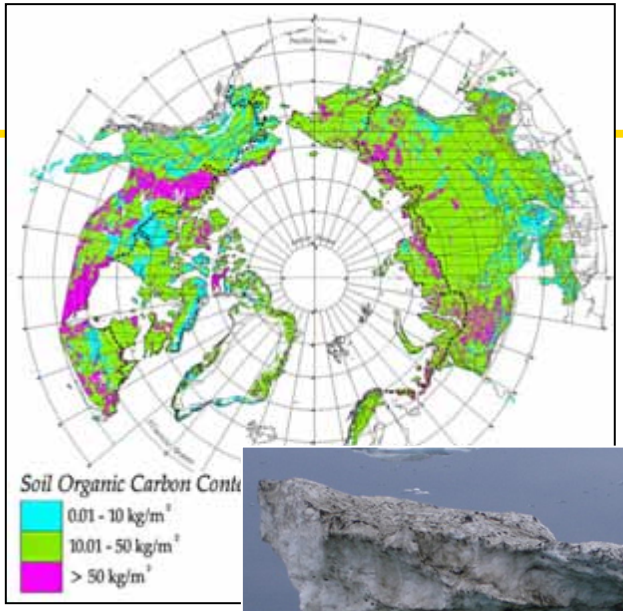
In addition to circulation, eddies are important for understanding currents, nutrients and biogeochemistry, sea ice edges, thermohaline circulation, etc.



(M. Maltrud et al)

Big Issues in High Latitudes

- Warming faster than the rest of the globe
- Sea ice extent shrinking, ice sheets melting, permafrost thawing
- Collects pollution from northern hemisphere
- Vast methane hydrate, oil and gas reserves
- Culturally and ecologically unique
- Of national security interest
- More carbon in permafrost than the rest of the global terrestrial carbon pool



LANL has a strong set of capabilities to apply to high latitude problems

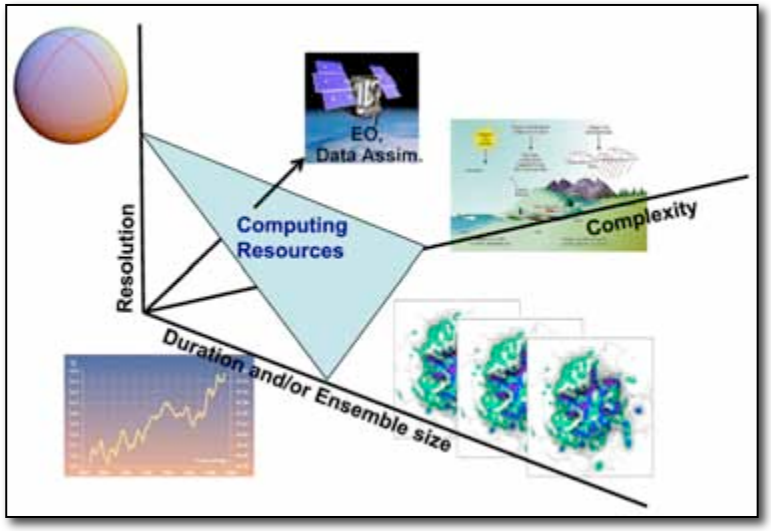
(Courtesy C. Wilson)

Enormous resources are required for predictive climate simulations

- **Finer resolution**
  - Provide regional details (10,000x)
- **Higher realism or more complexity**
  - Add "new" science (100x)
    - Biogeochemistry
    - Ice-sheets
  - Up-grade to "better" science (100x)
    - Better cloud processes
    - Dynamics land surface
- **Scenario replication or ensembles (UQ)**
  - Range of model variability (10x)
- **Time scale of simulation**
  - Long-term implications (100x)

Resource tradeoffs

Image courtesy of James Kinter (Center for Ocean-Land-Atmosphere Studies)



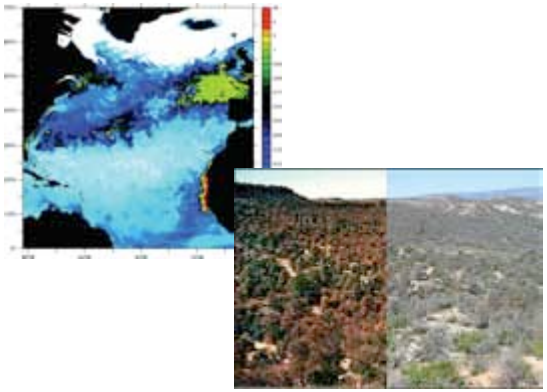
It is essential that computing power be increased substantially (by a factor of 1000), and scientific and technical capacity be increased (by at least a factor of 10) to produce weather and climate information of sufficient skill to facilitate regional adaptations to climate variability and change.
World Modeling Summit for Climate Prediction, May, 2008

From Climate Science Workshop (11/08)

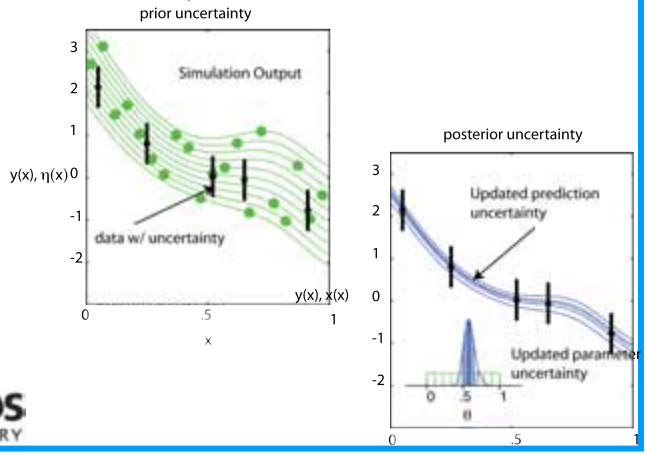
HPC Necessary but not Sufficient. LANL is Bringing Key Assets together: Co-Design for Energy and Climate Science: Impacts and Mitigations

Measurements & Analysis (Microbes to Satellites!)

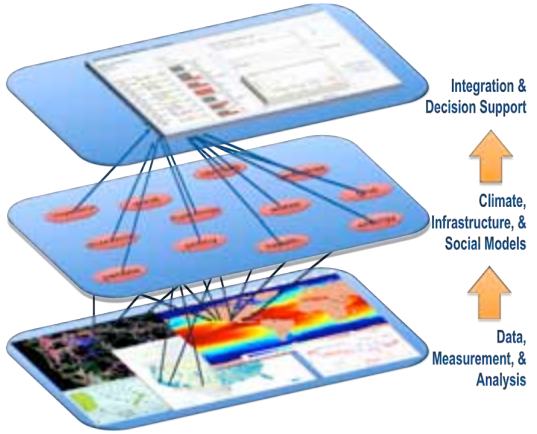
Climate and Modeling



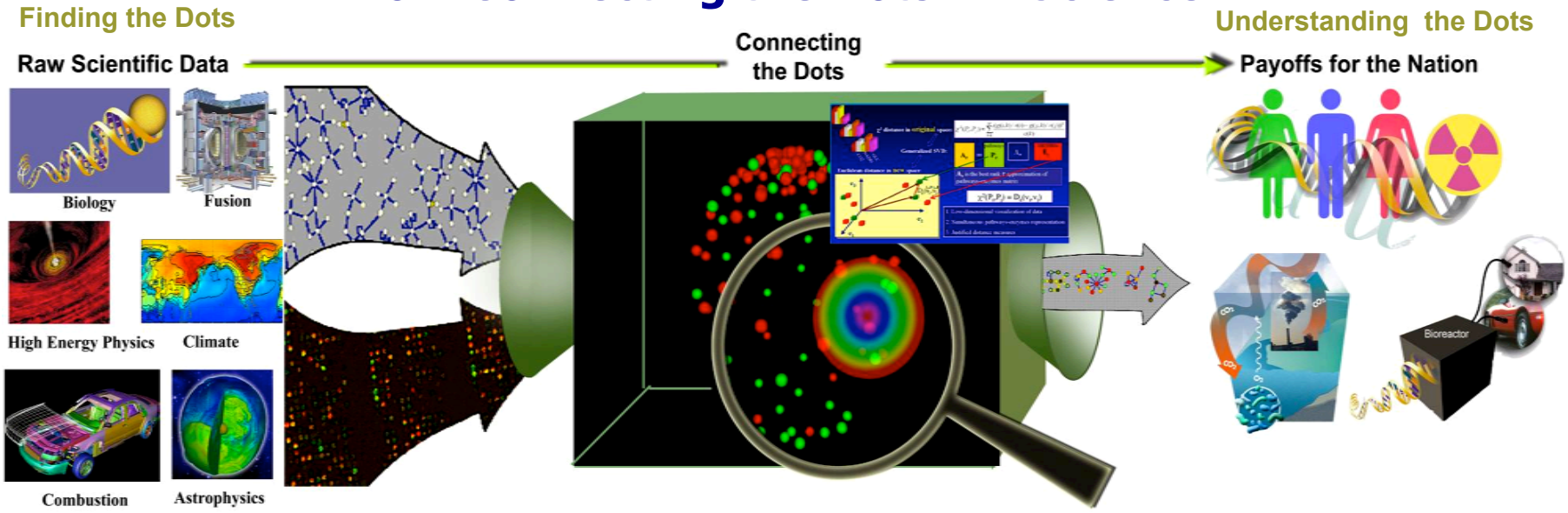
Uncertainty Quantification



Social, Energy, and Infrastructure Modeling



Information Science & Technology must become the Infrastructure for "Connecting the Dots" in Science



Sheer Volume of Data

Climate

Now: 20-40 Terabytes/year

5 years: 5-10 Petabytes/year

Fusion

Now: 100 Megabytes/15 min

5 years: 1000 Megabytes/2 min

Advanced Mathematics and Algorithms

- Requires high-performance computing, advanced theory modeling, data curation
- Huge dimensional space
- Combinatorial challenge
- Complicated by noisy data

Providing Predictive Understanding

- Produce hydrogen-based energy
- Stabilize carbon dioxide
- Clean and dispose toxic waste

Office of Science
U.S. DEPARTMENT OF ENERGY
Los Alamos NATIONAL LABORATORY
EST. 1943

c.f. Raymond L. Orbach, DOE Undersecretary for Science
2006 AAAS Annual Meeting

e.g., Visualization and Analysis of Massive (including Streaming) Data

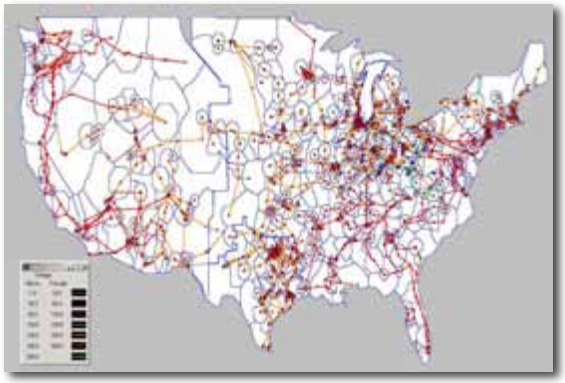
- **LANL exploring "Middle Ways" between numerically-intensive and data-intensive supercomputing**
  - Need for interactive scientific visualization of massive data quantities
- **Developing novel ways to use emerging computer hardware to enable real-time visualization and analysis of massive streaming datasets**
  - Use active storage and networks
  - Examples: materials, situational awareness, cyber, infrastructure, space . . .
- **Will enable a system that provides real-time:**
  - Processing (correlation) of incoming measurements
  - Analysis of correlated data to identify events of interest, their storage and use

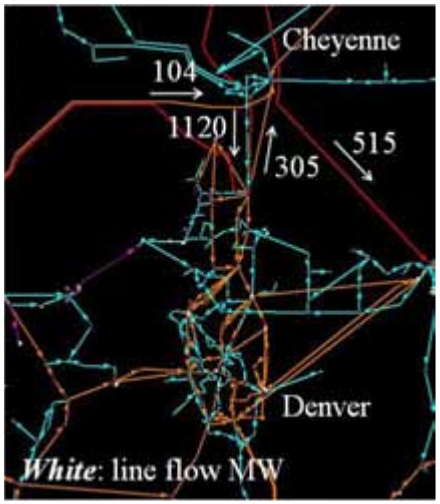
Immersion Visualization

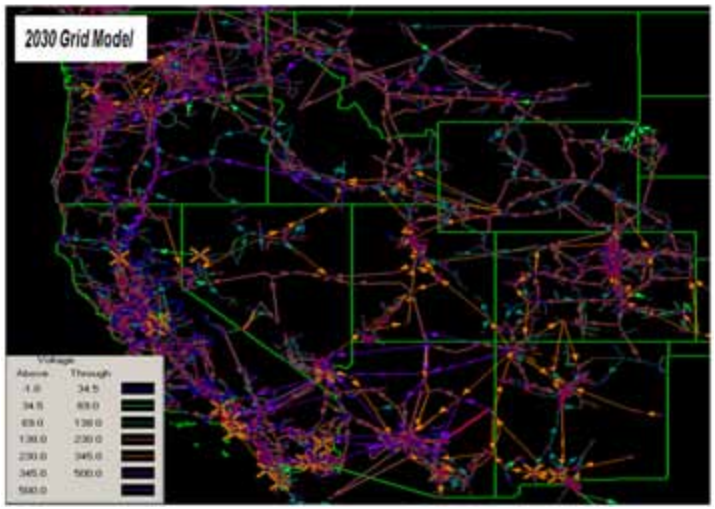
Energy Grid Challenges of the Future: a Complex Network

- Requires predictive simulation and rapid integration of new technologies for renewable generation, transmission, and storage: “Network S&T”
- Integration is needed to maintain grid stability.
- Cost-effective investment requires predictive simulation.

LANL develops energy infrastructure models to understand impacts and address power options for insertion of renewable and nuclear energy.

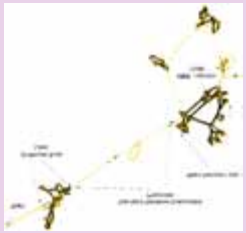






(M. Chertkov et al)

The LANL Cyber Systems Program
An Integrated Set of Technologies and Solutions



Data Intensive Computing

Multi-Domain Analysis, Classification & Detection

Multi-Scale Cyber Experimentation & Validation

Non-Traditional & Multi-Disciplinary Cyber Science

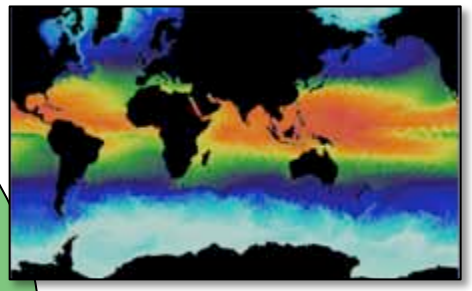
Foundational Cyber Technologies

- ***Advanced Threat Analysis, Detection, and Response Tools***
- ***Mobile Cyber Platform Solutions***
- ***Cyber Operation & Decision Support Frameworks***
- ***Experiential Cyber Training***

Differentiating Solutions

(A. Kent et al)

Summary: The Next Decade will be a Perfect Storm of Opportunity: Understanding, Prediction and Management



Simulations will become a critical component of decision making

Mission

Transformational technologies at all scales, including exascale

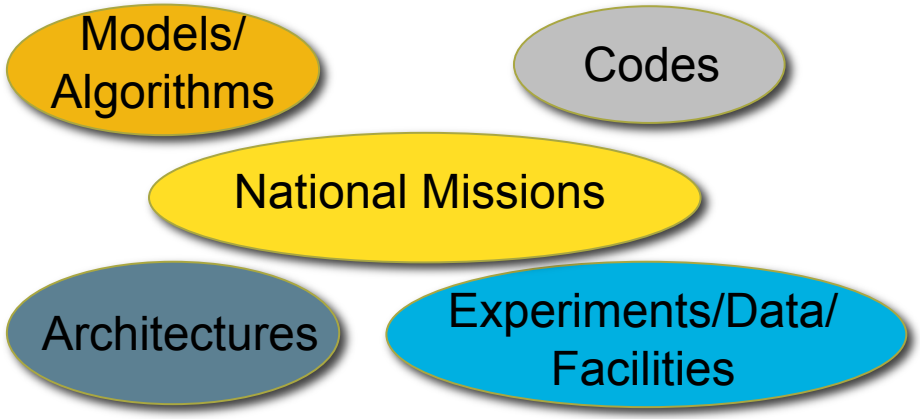
Computational science

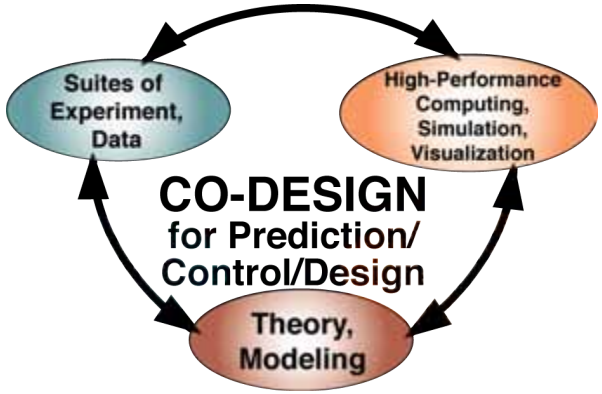
Game-changing facilities are coming on-line

Experimental science

Los Alamos NATIONAL LABORATORY EST.1943

"Co-Design" Can Define a Future with Maximum Impact: A national S&T management challenge





What should a next-generation user facility look like? Beyond "cottage industries"?

- **Resetting integration and collaboration framework for transformational S,T & E at Science & Mission Frontiers (DOE: SciDAC, Hubs, Co-Design Centers…)**
- **LANL opportunities being developed: NW Predictive Capability Framework, Energy–Climate, Astroinformatics, Environmental Management, Cyber,…MaRIE…**

(Interdisciplinary teams, Agile codes, IS&T tools, Analysis & Visualization of massive (streaming) data…)

DOE (SC, NNSA, Programs) has a full spectrum of assets for this future
: Integrating National Assets for Discovery, Prediction, Control, Design